

Topology Changes and Quantum Phase Transition in Spin-Chain System

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The standard Landau-Ginzburg scenario of phase transition is broken down for quantum phase transition. It is difficult to find an order parameter to indicate different phases for quantum fluctuations. Here, we suggest a topological description of the quantum phase transition for the XY model. The ground states are identified as a specialized $U(1)$ principal bundle on the base manifold S^2 . And then different first Chern numbers of $U(1)$ principal bundle on the base manifold S^2 are associated to each phase of quantum fluctuations. The particle-hole picture is used to parameterized the ground states of the XY system. We show that a singularity of the Chern number of the ground states occurs simultaneously with a quantum phase transition. The Chern number is a suitable topological order of the quantum phase transition.

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INTRODUCTION

A classical phase transition brings about a sudden change of the macroscopic properties of a many-body system while varying smoothly temperature. The appearance of a singularity on canonical thermodynamic function is a signature of a phase transition. Furthermore, theorem of Lee and Yang relates the properties of the zeros of the grandcanonical partition function in the complex fugacity plane to singularity of the corresponding thermodynamic function. In the Landau-Ginzburg scenario of phase transition, the symmetry breaking described by order parameters indicates a phase transition. P. W. Anderson believed that the interaction of the twin concepts of broken symmetry and of adiabatic continuity is the logical core of many-body physics[1].

However, some systems found fails to fall in the standard framework of phase transition. Such as different fractional quantum Hall states have the same symmetry but contains a completely new kind of order (topological order). The classical statistical systems are described by positive probability distribution functions of infinite variables while fractional quantum Hall states are described by their ground state wave functions which are complex functions of infinite variables. Quantum states contain a kind of order that is beyond symmetry characterization[2, 3].

For a many-body system at absolute zero temperature, all thermal fluctuations are frozen out and quantum fluctuations retained only. These microscopic quantum fluctuations can drive a macroscopic phase transition. This phenomenon, known as quantum phase transition (QPT), corresponds dramatic changes of ground states due to a small variation of external parameters[4]. It is ascribed to the interplay between different orderings associated to competing terms in the Hamiltonian of the systems. QPT has attracted considerable significance because of its association with condensed matter physics and quantum information, though it is still difficult to identify a proper parameter for indicating the

symmetry breaking in the QPT systems.

Recently, tools in theory of quantum information have been used to characterize the critical points of QPTs. The connections between QPTs and quantum entanglement[5] was explored. Geometric phase was used also as an indicator of QPTs[6]. QPTs can be studied systematically by means of differential geometry of projective Hilbert space[7]. Geometric quantities of a quantum many body system undergoing a QPT (in the thermodynamic limit) display discontinuous features abruptly. In particular, critical behavior corresponds properly to a singularity of the metric equipped in parameter manifold of the ground states of the quantum many-body systems. Moreover, the metric obeys scaling behavior in the vicinity of a QPT. This differential geometry approach stimulates investigations of QPTs from a quite different point of view.

In this Letter, within the framework of differential geometry description of the QPTs, we develop a connection between a singularity of the Chern number (a simple topological order) associated with the ground states of the XY model and a transition among different phases caused by quantum fluctuations. The ground states of the XY system after rotating are parameterized by three parameters, the anisotropy γ , rotating angle ϕ and the magnetic field λ . For the case of $\gamma \in [0, \infty)$ (the other case of $\gamma \in (-\infty, 0]$ can be discussed in the same manner), the ground states can be identified as a specified $U(1)$ principal bundle parameterized by λ on the base manifold $S^2_{\phi\gamma}$. We calculate the first Chern number (a function of the magnetic field λ) for the ground states on the base manifold $S^2_{\phi\gamma}$. It is found that different Chern numbers of $U(1)$ principal bundle on the base manifold $S^2_{\phi\gamma}$ are associated to each phase of quantum fluctuations. The particle-hole picture of Lieb, Schultz and Mattis[8] is used to parameterized the ground states of the XY system. We show that a singularity of the Chern numbers of the ground states occur simultaneously with a quantum phase transition. The Chern number is suggested as a suitable topological order of QPTs.

DIFFERENTIAL GEOMETRIC DESCRIPTION

QPTs behave distinctively from temperature-driven critical phenomena as a consequence of competition between different parameters, $\Lambda \in \mathcal{M}$ (the parameter manifold), in the Hamiltonian $H(\Lambda)$ of the system. For different Hamiltonians, these parameters describe different basic interactions, respectively. QPTs take place for a parameter region where the energy levels of the ground state and the excited state cross or have an avoided crossing. The ground state $|\psi_0(\Lambda)\rangle$ gives a mapping of the parameter manifold \mathcal{M} onto the projective Hilbert space. In the projective Hilbert space, one can define naturally a metric, the Fubini-Study metric[9]

$$ds^2 = \langle d\psi_0 | d\psi_0 \rangle - \langle d\psi_0 | \psi_0 \rangle \langle \psi_0 | d\psi_0 \rangle. \quad (1)$$

In fact the complex Hermitean tensor[7]

$$\mathcal{G}_{\mu\nu} = \langle \partial_\mu \psi_0 | \partial_\nu \psi_0 \rangle - \langle \partial_\mu \psi_0 | \psi_0 \rangle \langle \psi_0 | \partial_\nu \psi_0 \rangle, \quad \mu, \nu = 1, \dots, \dim \mathcal{M}, \quad (2)$$

can be introduced. The real component of \mathcal{G} is just the Fubini-Study metric expressed in the parameter space.

Generally, the definition of the Fubini-Study metric on the ground states can be extended to arbitrary normalized eigenstates $|\psi_n(\Lambda)\rangle$ of $H(\Lambda)$ with eigenvalue $E_n(\Lambda) = \langle \psi_n(\Lambda) | H(\Lambda) | \psi_n(\Lambda) \rangle$, and $d^2(\psi_n, \psi_n + d\psi_n) = \sum_{m \neq n} |\langle \psi_m | d\psi_n \rangle|^2$. By using the differential of the eigenstate equation $d([H - E_n]|\psi_n\rangle) = 0$, we get

$$d^2(\psi_n, \psi_n + d\psi_n) = \sum_{m \neq n} \frac{\langle \psi_m | dH | \psi_n \rangle \langle \psi_n | dH | \psi_m \rangle}{(E_m - E_n)^2}. \quad (3)$$

For the ground state, we can rewrite the complex Hermitean tensor \mathcal{G} as

$$\mathcal{G} = \sum_{m \neq 0} \frac{\langle \psi_m | dH | \psi_0 \rangle \langle \psi_0 | dH | \psi_m \rangle}{(E_m - E_0)^2}, \quad (4)$$

where E_0 and E_m are the energy of the ground state and excited state respectively, and the summation runs over all excited states $|\psi_m\rangle$ ($m = 1, 2, \dots$) of the system.

In the thermodynamic limit, QPTs take place where the energy gap between the ground state and the first excited state is vanishing for some specific parameters region. This is reflected in (4) where the denominator is vanishing and \mathcal{G} is divergent, resultantly.

The real component of \mathcal{G} induces a Riemannian metric in parameter manifold which behaves singularly while parameters approaching critical points. This property of induced metric in the parameter manifold has been investigated in detail for various models[7]. Here we focus on imaginary component of the complex Hermitean tensor $\mathcal{G}_{\mu\nu}$,

$$F_{\mu\nu} = \langle \partial_\mu \psi_0 | \partial_\nu \psi_0 \rangle - \langle \partial_\nu \psi_0 | \partial_\mu \psi_0 \rangle. \quad (5)$$

$F_{\mu\nu}$ is the Berry curvature two-form[10]. The ground state is a $U(1)$ principal bundle on the parameter manifold \mathcal{M} . The principal bundle can be classified by topological parameters. This, in fact, gives an explicit clarification of the configurations of ground states for a kind of general systems. Crossing of phase boundary on the parameter space corresponds to a singularity of the curvature two form $F_{\mu\nu}$. It is natural to expect that different winding numbers of the $U(1)$ principal bundle can be associated to different quantum phases.

THE GROUND STATE OF THE XY MODEL

In what follows, we present our arguments through the familiar XY model. The quantum XY model is a one dimensional spin-1/2 chain with nearest-neighbor interaction. The Hamiltonian of the model is described by

$$H(\gamma, \lambda) = -\frac{1}{2} \sum_{j=1}^N \left(\frac{1+\gamma}{2} \sigma_j^x \sigma_{j+1}^x + \frac{1-\gamma}{2} \sigma_j^y \sigma_{j+1}^y + \lambda \sigma_j^z \right), \quad (6)$$

where σ_j^x , σ_j^y , σ_j^z represent Pauli matrices at j -th lattice site. The parameter γ denotes the anisotropy in the in-plane nearest-neighbor interaction, and λ is the transverse field applied in z direction.

Critical behavior occurs at magnetic field $\lambda = \pm 1$ for any value of γ and $\gamma = 0$ for the value of $\lambda \neq \pm 1$. The eigenstate and eigenenergy can be exactly calculated by means of diagonalizing the Hamiltonian[8]. The most important step is the Jordan-Wigner transformation which maps spin-1/2 degrees of freedom to spinless fermions.

For the purpose of investigating topology of the system, we introduce another Hamiltonian[6] $H(\phi, \gamma, \lambda) \equiv R(\phi)H(\gamma, \lambda)R^\dagger(\phi)$ of the model by rotating $R(\phi) = \prod_{j=1}^N \exp(i\phi\sigma_j^z/2)$ every spin in system around the z direction with an angle $\phi \in [0, \pi]$. The Hamiltonian can be diagonalized by a standard procedure. By making use of the Jordan-Wigner transformation

$$a_l = \left(\prod_{m < l} \sigma_m^z \right) \frac{\sigma_l^x + i\sigma_l^y}{2}, \quad (7)$$

one converts the spin operators into fermionic operators

$$\begin{aligned} H(\phi, \gamma, \lambda) = & -\frac{1}{2} \sum_{j=1}^{N-1} (a_{j+1}^\dagger a_j + a_j^\dagger a_{j+1} - \gamma e^{2i\phi} a_j a_{j+1} + \gamma e^{-2i\phi} a_j^\dagger a_{j+1}^\dagger) \\ & + \lambda \sum_{j=1}^N (a_j^\dagger a_j) + \frac{1}{2} \alpha (a_1^\dagger a_N - a_N^\dagger a_1) + \frac{1}{2} \alpha \gamma (e^{-2i\phi} a_1^\dagger a_N^\dagger - e^{2i\phi} a_N a_1) \\ & - \frac{N}{2} \lambda, \quad (8) \end{aligned}$$

where $\alpha = \prod_{j=1}^{N-1} (1 - 2a_j^\dagger a_j)$ and satisfies $\alpha^2 = 1$, as well as $[H, \alpha] = 0$. H and α are simultaneously diagonalizable with eigenvalue of $\alpha = \pm 1$. For large system, we may neglect boundary terms. The Fourier transformation gives

$$d_k = \frac{1}{\sqrt{N}} \sum_{l=1}^N a_l e^{-i2\pi lk/N}. \quad (9)$$

Making use of the Bogoliubov transformation

$$\begin{aligned} c_k &= d_k \cos \frac{\theta_k}{2} - i d_{-k}^\dagger e^{-2i\phi} \sin \frac{\theta_k}{2}, \\ c_k^\dagger &= d_k^\dagger \cos \frac{\theta_k}{2} + i d_{-k} e^{2i\phi} \sin \frac{\theta_k}{2}, \\ c_{-k} &= d_{-k} \cos \frac{\theta_k}{2} + i d_k^\dagger e^{-2i\phi} \sin \frac{\theta_k}{2}, \\ c_{-k}^\dagger &= d_{-k}^\dagger \cos \frac{\theta_k}{2} - i d_k e^{2i\phi} \sin \frac{\theta_k}{2}, \end{aligned} \quad (10)$$

we obtain the Hamiltonian in a diagonal form

$$H(\phi, \gamma, \lambda) = \sum_{k=-[N/2]}^{[N/2]} \Lambda_k \left(c_k^\dagger c_k - \frac{1}{2} \right), \quad (11)$$

where Λ_k is the dispersion relation of the collective excitation mode c_k^\dagger ,

$$\Lambda_k = \pm \sqrt{\left(\cos \frac{2\pi k}{N} - \lambda \right)^2 + \gamma^2 \sin^2 \frac{2\pi k}{N}}. \quad (12)$$

The angle θ_k is determined by $\cos \theta_k = (\lambda - \cos \frac{2\pi k}{N}) / |\Lambda_k|$ and the sign of Λ_k is arbitrary. It should be noticed that the adoption of the sign of the dispersion relation does not affect the diagonalization of the Hamiltonian, but makes ambiguity in defining the ground state of the system.

To solve the ambiguity, we first focus on the case of $\gamma = 0$. Note that the model is isotropic and diagonalized without performing a Bogoliubov transformation. The Hamiltonian is $H(\phi, 0, \lambda) = \sum_{k=-[N/2]}^{[N/2]} \left(\lambda - \cos \frac{2\pi k}{N} \right) d_k^\dagger d_k$. The ground state is of the form,

$$\begin{aligned} |\psi_0\rangle &= \prod_{k=-[N/2]}^{-(k_T+1)} |0\rangle \otimes \prod_{k=-k_T}^{k_T} |1\rangle_k \otimes \prod_{k=k_T+1}^{[N/2]} |0\rangle, \\ k_T &= \begin{cases} \left[\frac{N}{2\pi} \arccos \lambda \right], & |\lambda| \leq 1, \\ 0, & |\lambda| > 1. \end{cases} \end{aligned} \quad (13)$$

In the particle-hole picture of Lieb, Schultz and Mattis[8], the Fermi energy of ground states for the isotropic XY model is given by $\frac{2\pi k_T}{N} = \arccos \lambda$.

Another important case, where the sign of the dispersion relation is determined explicitly, is of $\gamma = \sqrt{1 - \lambda^2}$. The diagonalized Hamiltonian is of the form

$$\begin{aligned} H(\phi, \sqrt{1 - \lambda^2}, \lambda) &= \sum_{k=-[N/2]}^{[N/2]} \sqrt{1 - \gamma^2} \\ &\times \left(\frac{\lambda}{1 - \gamma^2} - \cos \frac{2\pi k}{N} \right) \left(c_k^\dagger c_k - \frac{1}{2} \right). \end{aligned} \quad (14)$$

The ground state $|\psi_0\rangle$ can be constructed as

$$|\psi_0\rangle = \prod_{k=-[N/2]}^{[N/2]} \left(\cos \frac{\theta_k}{2} |0\rangle_k |0\rangle_{-k} + i e^{-2i\phi} \sin \frac{\theta_k}{2} |1\rangle_k |1\rangle_{-k} \right), \quad (15)$$

where $|0\rangle_k$ denotes vacuum of d_k , and $|1\rangle_k = d_k^\dagger |0\rangle_k$. Generally, we can rewrite the Hamiltonian as

$$\begin{aligned} H(\phi, \gamma, \lambda) &= \sum_{k=-[N/2]}^{-(k_T+1)} |\Lambda_k| \left(c_k^\dagger c_k - \frac{1}{2} \right) \\ &- \sum_{k=-k_T}^{k_T} |\Lambda_k| \left(c_k^\dagger c_k - \frac{1}{2} \right) + \sum_{k=k_T+1}^{[N/2]} |\Lambda_k| \left(c_k^\dagger c_k - \frac{1}{2} \right), \end{aligned} \quad (16)$$

where we have used the notation

$$k_T \equiv \begin{cases} \left[\frac{N}{2\pi} \arccos \frac{\lambda}{1 - \gamma^2} \right], & \text{for } \left| \frac{\lambda}{1 - \gamma^2} \right| \leq 1 \\ 0, & \text{otherwise.} \end{cases}$$

c_k^\dagger creates a hole if $0 \leq \frac{2\pi|k|}{N} \leq \arccos \frac{\lambda}{1 - \gamma^2}$ for $\left| \frac{\lambda}{1 - \gamma^2} \right| \leq 1$. But c_k^\dagger creates a particle if $\pi \geq \frac{2\pi|k|}{N} > \arccos \frac{\lambda}{1 - \gamma^2}$ for $\left| \frac{\lambda}{1 - \gamma^2} \right| \leq 1$. In the case of $\left| \frac{\lambda}{1 - \gamma^2} \right| > 1$, no hole excitation mode exists. The corresponding ground state of the Hamiltonian $H(\phi, \gamma, \phi)$ is of the form

$$\begin{aligned} |\psi_0\rangle &= \prod_{k=-[N/2]}^{-(k_T+1)} \left(\cos \frac{\theta_k}{2} |0\rangle_k |0\rangle_{-k} + i e^{-2i\phi} \sin \frac{\theta_k}{2} |1\rangle_k |1\rangle_{-k} \right) \\ &\otimes \prod_{k=-k_T}^{k_T} \left(\cos \frac{\theta_k}{2} |1\rangle_k |1\rangle_{-k} - i e^{2i\phi} \sin \frac{\theta_k}{2} |0\rangle_k |0\rangle_{-k} \right) \\ &\otimes \prod_{k=k_T+1}^{[N/2]} \left(\cos \frac{\theta_k}{2} |0\rangle_k |0\rangle_{-k} + i e^{-2i\phi} \sin \frac{\theta_k}{2} |1\rangle_k |1\rangle_{-k} \right). \end{aligned} \quad (17)$$

In the case of $\lambda = 0$, the Fermi energy reduces to $\pi/2$. This is just the scenario described by Lieb, Schultz and Mattis[8].

TOPOLOGICAL ORDER AND QUANTUM PHASE TRANSITION

There are three parameters λ , γ and ϕ in the Projective Hilbert space \mathcal{PH} of the ground states. We note the fact

that the Hamiltonian $H(\phi, \gamma, \lambda)$ is π periodic in ϕ . The projective Hilbert space \mathcal{PH} can be viewed as a $U(1)$ principal bundle parameterized by λ on the base manifold $S^2_{\phi\gamma}$ ($\gamma \in [0, \infty)$, $\phi \in [0, \pi)$).

The curvature tensor of the principal bundle on the base manifold $S^2_{\phi\gamma}$ is of the form

$$\begin{aligned} F_{\phi\gamma} &= \left\langle \frac{\partial\psi_0}{\partial\phi} \middle| \frac{\partial\psi_0}{\partial\gamma} \right\rangle - \left\langle \frac{\partial\psi_0}{\partial\gamma} \middle| \frac{\partial\psi_0}{\partial\phi} \right\rangle \\ &= \frac{2i}{\pi} \left(\int_{2\pi k_T/N}^{\pi} d\alpha \frac{\gamma \sin^2 \alpha (\lambda - \cos\alpha)}{[(\cos\alpha - \lambda)^2 + \gamma^2 \sin^2 \alpha]^{3/2}} \right. \\ &\quad \left. - \int_0^{2\pi k_T/N} d\alpha \frac{\gamma \sin^2 \alpha (\lambda - \cos\alpha)}{[(\cos\alpha - \lambda)^2 + \gamma^2 \sin^2 \alpha]^{3/2}} \right). \quad (18) \end{aligned}$$

Here the sum in the above equation has been replaced by integration, as in the following, we will discuss the topological changes caused by QPT's in the thermodynamic limit.

The first Chern number[11] of the ground states on the base manifold $S^2_{\phi\gamma}$ is[12]

$$C_1(\lambda) = \frac{i}{2\pi} \int_0^{\pi} d\phi \int_0^{\infty} d\gamma F_{\phi\gamma} = \begin{cases} -1, & \text{for } 0 \leq \lambda < 1, \\ -2, & \text{for } \lambda = 1, \\ 0, & \text{for } \lambda > 1. \end{cases} \quad (19)$$

According to the result (19) on the first Chern numbers of the ground states, we can draw a phase diagram for the XY model. It is clear to see that it is the same with the QPT diagram. Thus, the Chern number can be really employed as a tool in describing the QPTs.

CONCLUSIONS AND PERSPECTIVES

The result obtained in the thermodynamic limit shows clearly that the QPTs can be associated with a change in the topology of the ground states. The topological description of the QPT's presented here shares remarkable similarity to the topological order picture of the integer quantum Hall effect[2, 13], where Hall conductance is explained as a topological invariant. Further investigations of the similarities between QPT's in the spin chain and quantum Hall effect may be interesting and we hope they will benefit from each other.

Recently, quantum entanglement is intensively studied in quantum many-body systems[5]. The entanglement changes drastically while a parameter varying smoothly and the system crossing through critical points. This phenomena promotes the understanding of the relation between the entanglement and QPTs. It also has been suggested that the classical phase transition might has its deep origin in topological change of configuration space[14]. It is nature to wish a same topological perspective on the phase transition of both classical and

quantum many body systems. Further investigations on the relation between them is worthwhile.

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- [1] P. W. Anderson, *Basic Notions of Condensed Matter Physics*, The Benjamin-Cummings Publishing Company, Inc. London, 1984.
- [2] Q. Niu, D. J. Thouless and Y. S. Wu, Phys. Rev. B³¹, 3372 (1985).
- [3] X. G. Wen and Q. Niu, Phys. Rev. B⁴¹, 9377 (1990).
- [4] S. Sachdev, *Quantum Phase Transitions*, Cambridge University Press, Cambridge, England, 1999.
- [5] A. Osterloh, L. Amico, G. Falci, and R. Fazio, Nature 416, 608 (2002); T. J. Osborne and M. A. Nielsen, Phys. Rev. A⁶⁶, 032110 (2002); G. Vidal, J. I. Latorre, E. Rico, and A. Kitaev, Phys. Rev. Lett. 90, 227902 (2003); L. A. Wu, M. S. Sarandy, and D. A. Lidar, Phys. Rev. Lett. 93, 250404 (2004); T. R. de Oliveira, G. Rigolin, M. C. de Oliveira, and E. Miranda, Phys. Rev. Lett. 97, 170401 (2006).
- [6] A. C. M. Carollo and J. K. Pachos, Phys. Rev. Lett. 95, 157203 (2005); S. L. Zhu, Phys. Rev. Lett. 96, 077206 (2006); A. Hamma, quant-ph/0602091.
- [7] P. Zanardi, P. Giorda, and M. Cozzini, Phys. Rev. Lett. 99, 100603 (2007); L. CamposVenuti and P. Zanardi, Phys. Rev. Lett. 99, 095701 (2007).
- [8] E. Lieb, T. Schultz, and D. Mattis, Ann. Phys. (N.Y.) 16, 407 (1961).
- [9] S. Kobayashi and K. Nomizu, *Foundations of Differential Geometry*, Interscience, New York, 1969; J. Anandan and Y. Aharonov, Phys. Rev. Lett. 65, 1697 (1990).
- [10] M.V. Berry, Proc. R. Soc. London A³⁹², 45 (1984); Y. Aharonov and J. Anandan, Phys. Rev. Lett. 58, 1593 (1987); *Geometric Phases in Physics*, edited by A. Shapere and F. Wilczek, World Scientific, Singapore, 1989.
- [11] Y. Choquet-Bruhat, C. DeWitt-Morette, and M. Dillard-Bleick, *Analysis, Manifolds and Physics*, North-Holland, Amsterdam, 1982.
- [12] The numerical computation of the Chern numbers shows amount of deviation from the data near critical points because of singularity behavior of the curvature.
- [13] D. J. Thouless, M. Kohmoto, M. P. Nightingale and M. den Nijs, Phys. Rev. Lett. 49, 405 (1982); J. E. Avron and R. Seiler, Phys. Rev. Lett. 54, 259 (1985).
- [14] L. Casetti, M. Pettini, and E. G. D. Cohen, Phys. Rep. 337, 237 (2000); L. Casetti, M. Pettini, and E. G. D. Cohen, J. Stat. Phys. 111, 1091 (2003); L. Caiani, L.

Casetti, C. Clementi and M. Pettini, Phys. Rev. Lett. **79**, 4361 (1997); R. Franzosi, M. Pettini, and L. Spinelli, Phys. Rev. Lett. **84**, 2774 (2000); M. Kastner, Rev. Mod. Phys. **80**, 167 (2008).